

Photoelectronic Properties of Thiophene-Vinylene Derivatives with Phthalimide Groups in Both Terminals

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Abstract

We synthesized two novel thiophene-vinylene derivatives with phthalimide groups in both terminals. Thiophene-vinylene skeleton was effective to increase IP and to decrease optical band gap, meanwhile, introduction of phthalimide groups lowered ionization potential value (IP), meanwhile, thiophene-vinylene was effective to increase IP and to decrease optical band gap.

1. Introduction

Soluble-type semiconductor materials have much attention because their possibilities for printable processes of electronic devices such as thin film transistors, electroluminescent devices, photovoltaics, etc.[1,2] With regard to materials, fullerenes and their derivatives, such as [6,6]-phenyl C61 butyric acid methyl ester (PC61BM) and PC71BM, have been the dominant n-type semiconductors in organic electronic devices,[3,4] because of their large electron affinity, high electron mobility,[5,6] and the development of new synthetic routes toward soluble fullerenes.[7]

However, fullerenes have a few disadvantages, such as weak absorption in the visible spectrum compared to typical donor polymers, high-cost production and purification,[8,9] and an electron affinity that is too large with respect to the ionization potential of number of donor polymers, resulting in low open-circuit voltages (Voc).[10] In terms of tuning the properties of the fullerene derivatives, especially photoelectronic properties, it is not easy to prepare the fullerene derivatives with the desired photoelectronic properties. Meanwhile, organic n-type semiconductors are potentially promising because they have a high degree of freedom for the materials design.

Examples of the promising non-fullerene n-type semiconductors for application have been reported and reviewed. With regard to the skeleton, many researchers employed fused ring structures. However, the fused ring structures are likely to be insoluble due to their wide plane structures. On the other hand, aromatic vinylene skeleton shows a long conjugated length and has good miscibility.

Phthalimide groups have been known as electron withdrawing, recently, there have been reports on soluble semiconductors introduced with them.

We synthesized two novel organic compounds that have

thiophene-vinylene skeleton and phthalimide groups in both terminals, here, report characteristics of these compounds.

2. Experimental section

Material synthesis

Two compound were synthesized by the Heck reaction of 4-vinyl-N-octylphthalimide with selected dibromothiophene derivatives.[11,12]

Evaluation of characteristics.

Photoelectron spectra were recorded under the reduced pressure on an ultraviolet photoelectron spectrophotometer. Optical band gaps were determined from UV-vis absorption onset in thin films.

3. Result and discussion

Figure 1 shows the chemical structures of two compounds prepared in this study.

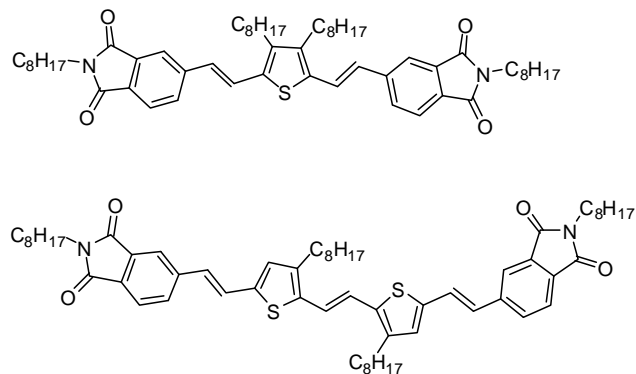


Fig. 1 Chemical structures of the compounds prepared in the present study. Upper, T-1-2; lower, T-2-2.

Figure 2 shows energy level diagram showing HOMO and LUMO levels of two compounds. HOMO level of T-1-2 was -6.12 eV suggesting that T-1-2 acts as an n-type semiconductor. Since a thiophene ring is electron-donating, this demonstrates that the phthalimide group functions as a marked electron-withdrawing group. Meanwhile, T-2-2 showed the higher HOMO level of -5.64 eV than T-1-2. The introductions of thiophene ring and conjugated double bond enhanced the HOMO level. The optical band (ΔE_g) of T-2-2 was 1.85 eV that was less than that of T-1-2 at 2.20 eV.

This indicates that the conjugated area was extended by the introduction of thiophene ring and double bond.

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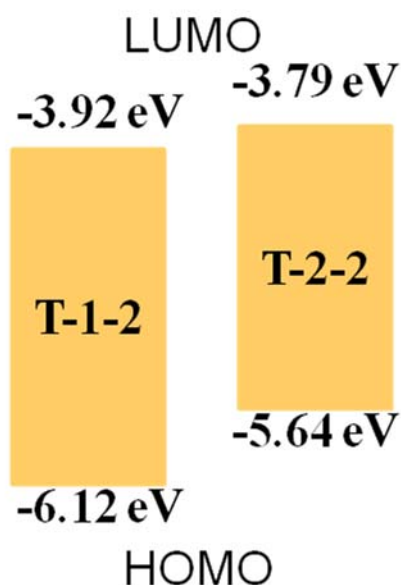


Fig. 2 Energy level diagram showing HOMO and LUMO levels of two compounds.

3. Conclusions

We synthesized two novel organic compounds that have thiophene-vinylene skeleton and phthalimide groups in both terminals. T-1-2 showed the low IP of -6.12 eV suggesting that it acts as the n-type semiconductor. The IP of T-2-2 was -5.64 eV, and higher than that of T-2-2.

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